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DEPARTMENT OF NATURAL RESOURCES
AND ENVIRONMENTAL CONTROL
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November 15, 1991

Mr. Randy Sturgeon (3HW25)
Enforcement Project Manager
U.S. EPA, Region III
841 Chestnut Building
Philadelphia, PA 19107

Subject: DNREC Review of Draft Risk Assessment DuPont-Newport Site (Human Health Evaluation) October 14, 1991

Dear Mr. Sturgeon:

DNREC has completed its evaluation of the referenced document. The Department's main concern rests with the evaluation of future risk from ingestion of groundwater from the Potomac Formation Aquifer. The Department does not believe that sufficient information has been provided from the groundwater modeling undertaken to characterize future risk to receptors drinking groundwater derived from the Potomac Formation Aquifer. The following briefly discusses the outstanding deficiencies noted from this groundwater modeling effort.

1. The modeling effort was conducted on a limited number of contaminants (i.e. Antimony, Arsenic, Barium, Beryllium, Cadmium, PCE, TCE, and zinc, see Table D-1). However, in the computational assessment of future risk contaminant values derived from the modeling effort were included with contaminant values derived from the remedial investigation (i.e. compare Appendix F. Future ingestion of Groundwater with Table 2-9 Summary of Analytical Data for Potomac Formation Groundwater DuPont - Newport site).

   In other words, DuPont has selectively chosen a limited number of contaminants to model. The modeled results were then included with the analytical data from Table 2-9 to develop future risk. This type of assessment is clearly inconsistent. DuPont should either model for all contaminants and evaluate future risks, or use all the relevant data from Table 2-9, but not some from both!

2. DuPont modeled the contaminants present in the Potomac Formation Aquifer as behaving a slug (i.e. a discontinuous/discrete plume of contaminated groundwater). I do not believe this assumption is valid. Review of the analytical data from subsurface borings of the Potomac Formation (at this interval) indicates that the soil is contaminated. The soil will serve as a continuous source of contamination to the Potomac Aquifer. Therefore, DuPont should revise their model to assume a continuous source of contamination.

3. DuPont's model assumes an area of source contamination. As the source moves along a unidirectional flow path to the receptor attenuation / dilution presumably occurs. The model does not account for contaminant contributions from areas outside the source area (or at least no mention is provided). With respect to contaminant plume dilution/attenuation, it may not be reasonable to presume that contaminant concentration levels in the plume would diminish to the levels prescribed by the model. DuPont should evaluate and provide information regarding the solubilities of individual contaminants in water. Have some of the contaminants reached supersaturation in the groundwater? What is the cation exchange capacity of soils? Can the soils accept more metal cations from solution?

4. The model assumed one direction of flow. Based upon the hydraulic head data gathered from the RI, it is clear that vertical and horizontal components of flow are present in the Potomac Formation Aquifer. DuPont should provide an explanation of the impact of vertical components of flow on the modeled results.

5. There is no information about the input parameters and how were they determined. The information is critical for evaluation of a modeling procedure.

6. There is no discussion about the uncertainties and limitations of the model used in this site. How confident does the modeler feel about the results of the model?

7. The locations of wells WW1 through WW12 are not provided. According to DuPont, these wells were the conduits for contaminant migration into the Potomac Aquifer. It is important to know where these wells are/were "located".

In addition to the aforementioned comments, I have enclosed a copy of the Superfund Branch's "Guidance on the Use of Groundwater Models". This guidance outlines the documentation requirements for groundwater modeling submissions performed at state Superfund sites. In light of the comments presented, I strongly recommend that DuPont be required to submit documentation in support of their groundwater modeling effort which at least meets these standards.

Sincerely,

Karl F. Kalbacher

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Environmental Program Manager
Superfund Branch

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Enclosure

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GUIDANCE ON THE USE OF GROUNDWATER MODELS

Draft

Prepared By:
The Delaware Department of Natural Resources
and Environmental Control, Superfund Branch
July, 1991

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1. INTRODUCTION

The use of groundwater models (computer simulation codes) in support of the planning and decision-making process in the management of groundwater has gained widespread acceptance in both government and industry. Groundwater models, when used appropriately, have proven to be a viable method in predicting contaminant transport, locating areas of potential environmental risk, and assessing possible remediation/corrective actions (van der Heijde, 1990).

The effective and appropriate application of groundwater models is, however, a qualitative procedure. As van der Heijde (1990) states, "its a combination of science and art. A successful model application requires a combination of knowledge of scientific principles, mathematical methods, and site characteristics paired with expert insight into the modeling process".

Owing to the inherent difficulties associated with simulating flow of groundwater and the transport of contaminants, the Superfund Branch of the Delaware Department of Natural Resources and Environmental Control (hereafter referred to as the Department) has developed this guidance document to provide technical standards on the use of groundwater models at state Superfund sites. In addition to providing technical standards, this guidance shall also serve to effectuate consistent documentation when models are used to support decisions at sites regulated by the Department.

2. PURPOSE

This guidance document focuses on the key issues in the selection, use and evaluation of groundwater modeling codes. The principle objectives of this guidance are to ensure that:

1) Selection of groundwater models is appropriate for the existing hydrogeologic conditions being modeled,
2) Model derived solutions acceptably match field observedvalues,
3) Quality controls in the modeling process are implemented, and
4) Results from the modeling process are critically evaluated and reported.

3. SCOPE

The aforementioned objectives apply principally to modeling undertaken to characterize groundwater flow and contaminant transport, estimate future concentrations and locations of contaminants in groundwater for analysis of risk, and support remedial decisions. In support of these decision-making processes, the standards in this guidance have been developed for modeling applications undertaken only after detailed field assessments of groundwater flow and contaminant transport have been conducted, and data necessary for calibrating the groundwater model have been collected.

These standards are limited to modeling of groundwater flow and contaminant transport in saturated porous media. Modeling of fracture flow or other complex systems is not addressed in this guidance document due to the inherent complexity of groundwater flow and contaminant transport in crystalline rocks. Modeling of multiple fluid phases such as air and water or immiscible organic chemicals and water is not part of the scope of this guidance.

The standards below pertain strictly to numerical computer models designed to simulate groundwater flow and contaminant transport. Heat transport and deformation models are not included in this guidance.

4. HYDROGEOLOGIC SITE CHARACTERIZATION

4.A CONCEPTUAL MODEL

The subsurface environment of groundwater is characterized by a complex interplay of physical, geochemical and biological forces that govern the release, transport and fate of a variety of chemical substances. To properly assess and predict the effect of groundwater contamination at a given site, a conceptual model needs to be developed. The conceptual model should explain all system stresses, boundaries, sources and sinks, and should present a clear, defensible understanding of the physics and chemistry of flow and transport in the system. A thorough understanding of the flow system is a prerequisite for successful transport simulations.

To provide an approximation of site specific groundwater flow and contaminant transport conditions, data used to construct the simulation and calibrate the model must be from site specific measurements. Detailed information about the nature of the suspected contaminants, the volume of contaminants disposed and released, and the time period over which contaminants were released is needed. The site investigation must address among other things the controls on contaminant migration, including the geology, soil, microbiology, geochemical interactions, and mass flow of contaminant to the water table (Groundwater, Handbook EPA/625/6-87/016 - March, 1987). Measurements of parameters must be taken in a manner that ensures they are representative of field conditions, and the density of measurements must accurately depict the distribution of aquifer properties, groundwater head, and contaminant concentrations. (Draft - Technical Standards for the Mathematical Modeling of Groundwater Flow and Contaminant Transport at Hazardous Waste Sites, State of California, Department of Health

Services, March, 1990).

Specific data which need to be evaluated and incorporated as appropriate into the conceptual model are:

1) Determination of hydraulic conductivity (ies) of hydrogeologic units at the modeled site.

2) Determination of the thickness of all geologic units of interest at the modeled site.

3) Description of the pertinent physical/chemical properties of hydrogeologic units/layers relative to the types of contaminants present. Particular attention should be directed towards determining the effect hydrogeologic units have on contaminant transport (ie: cation exchange capacity, organic carbon content, etc.).

4) Identification of the lithology and structural characteristics of the subsurface including facies changes, solution channels, cross cutting structures, pinch out zones, etc.

5) Identification of sorting, cementation, and grain size distribution in hydrogeologic units.

6) Determination of the direction(s) of groundwater flow (including both horizontal and vertical components) in hydrogeologic units.

7) Identification of causes of seasonal/temporal, natural and artificially induced variations in groundwater flow. (i.e. off-site production well pumping, irrigation, changing land use patterns, waste disposal practices, surface water effects, impoundments, unlined ditches, etc.).

8) Identification of the nature of hydraulic interconnection between hydrogeologic units.

9) Calculation of water balance at the site.

10) Determination of hydrologic boundaries surrounding the modeled area of interest. The type of boundary shall be specified according to whether it is specified head, specified flux, or head-dependent flux.

11) Determination of sources of contamination within the modeled area of interest including spatial orientation, concentration gradients, and rate(s) of contaminant movement into hydrogeologic units of interest.

12) Determination of natural or background values of chemical species of interest.

13) Determination of water quality in sources and sinks in the area of interest.

14) Categorization of sources of contamination (ie: point source, non-point source, source of limited areal extent, continuous source, or slug).

15) Identification and evaluation of surface control structures / measures used to restrict the infiltration of contamination or rainfall into the subsurface.

16) Identification and evaluation of subsurface control structures used to reduce the migration of contaminants into the unsaturated or saturated zone.

The information collected during hydrogeologic site characterization must adhere to Department quality assurance/quality control specifications. Information regarding quality assurance procedures for field sampling and laboratory analysis, and guidance on performing hydrogeologic investigations is contained in the Hazardous Substance Cleanup Act Interim Regulations Guidance Document.

5. MODEL SELECTION

5.A RATIONALE

There are many types of models which can be used to simulate groundwater flow and solute transport systems. The majority of models have been devised to simulate particular hydrogeologic scenarios (ie: saltwater intrusion, regional aquifer analysis, groundwater pollution, groundwater / surface water interactions, etc.) Models which perform similar functions tend to utilize similar computational procedures. Each code is unique, however, and therefore the resultant product is also unique.

The appropriate selection of a model is critical to the overall success of the modeling project. The selection of a particular model should be based upon its ability to accurately represent the hydrogeologic system, and on its ability to address the hydrogeologic questions which motivated the model study. Models which are used in hydrogeologic settings for which they were not intended oftentimes result in inappropriate prediction and miscalculation (Mercer and Faust, 1986).

To provide guidance on model selection, the following procedures have been devised. Criteria to be used in the model selection process have been classified into three categories:

1) Model Applicability
2) Model Testing

3) Model Documentation.

5.A1 Model Applicability

The selection of a numerical model to simulate real groundwater systems requires that the code be designed to adequately represent conditions in the real system. The code must be capable of representing all major hydrologic and geochemical processes active at the site.
The model selected must be capable of adequately representing the flow system at the site. Models which are capable of representing flow in three dimensions are preferred by the Department. Technical justification needs to be provided if the flow system is modeled in less than three dimensions.

Transport processes are those processes by which substances move through porous media. These transport processes include diffusion, advection, and dispersion. All models will need to be able to solve for these transport processes. Any models which do not address any one of these transport processes in the code will need to provide written justification for excluding the process.

Transformation, as it relates to contaminants in the groundwater, is the change in the chemical or physical state of a contaminant through the interaction of the contaminant with the groundwater and sediment. Transformation processes generally result in a reduction in the concentration of the contaminant in the groundwater, but may increase the concentration of other species in the system. Transformation processes include volatilization, oxidation-reduction reactions, sorption, biodegradation, and hydrolysis reactions.

Transformation processes can greatly affect the prediction of contaminant concentrations. Therefore, technical justification will need to be provided should any one of the processes be excluded from the model.

5.A2 Model Testing

Model testing is a process of determining the validity of model prediction of conditions in the prototype system. This process generally involves model verification and model validation. Model verification assesses the accuracy of the algorithms used to solve the necessary governing equations. Model validation determines how well the model's theoretical foundation and computer implementation describe actual system behavior in terms of the "degree of correlation" between model calculations and independently derived observations of the cause and effect responses of the prototype groundwater system (Van der Heijde, 1987).

Both model verification and validation need to be provided within the modeling package. Although standards for verification can not be set because of the inherent differences which exist among models, the codes need to be tested against synthetic problem sets which have exact solutions. In addition, documentation will need to be supplied which documents that the model has undergone quality control analysis and is fully operational (ie: no errors in programming exist).

Model validation should be conducted over a full range of hydrogeologic conditions including conditions which are similar to the proposed site. The validation procedure should also include documentation on predetermined performance criteria.

5.A3 Model Documentation

Procedures to be followed regarding model documentation follow those outlined by El-Kadi (1983). Documentation shall include:

1) A brief description of the model, providing information identifying the model, the author (or the person who provides the support), the organization where the model was developed, the version number or updates (if any), the programming language, and a brief description of the model's intended use.

2) Engineering description, including the basic theory and the method of solution, and its limitations and underlying assumptions.

3) Program documentation describing program capabilities and limitations, and lists of input and output variables.

4) Documentation containing information on the structure of the program, and a discussion of the model computer code.

5) Peer review by independent, qualified modelers. The determination of modelers qualified to perform peer reviews shall be made by the Department on a case by case basis.

If any modifications are made to the code, documentation regarding the affect the changes have on the code must be supplied. In addition, the Department may request that a separate model testing program be conducted.

Proprietary models are not excluded from the model documentation requirements.

5.B MODEL CONFIGURATION

The model which is selected must be capable of addressing the principle hydrogeologic conditions and contaminant flow characteristics at the the site. The basis for this assessment shall come from the information provided in the hydrogeologic site characterization.

The use of three dimensional models is preferred. If two dimensional models are used, technical justification must be provided for simulating the system in reduced dimensionality.

The selected model must be capable of representing heterogeneities or anisotropies which normally exist in porous media. Technical justification will need to be supplied if the groundwater system is modeled as homogeneous and isotropic.

5.C MODEL BOUNDARIES

The groundwater modeling process provides for the use of both physical and artificial boundary conditions. Use of either or both of these types of boundary conditions is site dependent; however, justification will need to be provided for the type and placement of lateral and vertical boundaries. In addition, if any internal boundaries such as sources or sinks are included in the model, then justification for modeling this condition will need to be provided.

The location of boundaries relative to stresses induced in the modeled system can affect model calibration or model prediction. Sensitivity analyses will need to be conducted to determine the degree to which the modeled solution varies.

5.D GRID DESIGN

The design of the nodal or grid network is of critical importance in the modeling process. The orientation of the grid pattern may affect model output. Grids which are too coarse may result in a reduction in the accuracy of the model output. This effect is dependent on the resolution of the input data.

Ideally the orientation of the grid pattern should adhere to the following guidelines as amended from Mercer and Faust, 1986:

1) "Well" nodes should be located near pumping wells or near well fields.

2) Where there are large spatial changes in transmissivity or hydraulic head the nodes should be placed closer together.

3) The axes of the grid should be aligned parallel with the major directions of the hydraulic conductivity tensor.

4) Avoid grid patterns where large spacings are adjacent to small spacings.

The reasoning used in the development of the grid network is a necessary component in the modeling process. It provides insight into the modelers interpretation of the site hydrogeologic conditions. Therefore, a discussion of the rationale used to develop the network design must be included in the model submission.

5.E INITIAL INPUT PARAMETERS

The initial input parameters supplied to the numerical model need to be included in the submission of the model results. The values for these parameters should come from field measurements at the modeled site and should be presented in a tabular format.

The initial input parameters should be provided for steady state conditions. In the event that transient hydrologic conditions predate the initiation of modeling, then input parameters for transient conditions may be provided. The Department will assess the validity of transient hydrologic input parameters based upon data gathered from the hydrogeologic site characterization.

5.F CALIBRATION

Calibration is the process of adjusting input parameters in the model to acceptably match both the site specific hydrogeologic conditions as well as the spatial distribution of contamination. The calibration is a "fine tuning" process which requires considerable skill. Models can be inappropriately calibrated to simulate site specific conditions using unrealistic parameter values. Calibrated values should be within the range of values for the site. Therefore, it is critical that the appropriate rationale be provided in the model document submission to substantiate the assumptions/calibration values chosen to perform the calibration.

Procedures to be followed regarding model calibration documentation follow those outlined from California's Draft - Technical Standards for the Mathematical Modeling of Groundwater Flow and Contaminant transport at Hazardous Waste Sites. Documentation shall include:

1) A tabular listing of all parameter values used to produce the calibrated model. The listing should also include specific data point locations used to calibrate the model.

2) A presentation of model results versus field observed values. Potential head measurements and contaminant concentrations shall be presented in the form of contour maps of observed and simulated values.

3) The mass balance of water flow and contaminant mass (for transport models) shall be presented for the calibrated model.

4) A discussion of the rationale and assumptions used to adjust input parameters to achieve the final calibration.

5) A discussion of the criteria used to terminate the calibration process (ie: the definition of an adequate match between observed and modeled values).

5.G SENSITIVITY ANALYSIS

Sensitivity analysis is the process of characterizing the independent effects of changes in parameters on the behavior of the calibrated model (California's Draft - Technical Standards for the Mathematical Modeling of Groundwater Flow and Contaminant transport at Hazardous Waste Sites). Sensitivity analyses can indicate whether model response is affected by only small changes in parameter values. They can also indicate if there is some overriding control in the system which prevents the model from responding to changes in parameter values.

The importance of performing sensitivity analysis can not be overstated. Therefore, the Department will require that the model document submission include a detailed and thorough analysis of sensitivity on aquifer parameter values included in the model.

5.H VERIFICATION

The process of verifying a model entails comparing the calibrated data set to future independent field observed values. The basis for performing this assessment is twofold: 1) it re-evaluates the predictive capability of the model and 2) it allows for additional fine tuning to be conducted to the model.

Because the verifying process can only occur a considerable time after the calibrated model has been finalized, the Department can not require any documentation be provided in the initial model submission. However, should the model be used for predictive purposes with regard to remedial/corrective action decisions, then the Department shall require that model verification be conducted. The timetable for requiring model verification will be specified by the Department on a case by case basis.

Department requirements for model verification include:

1) A presentation in tabular form of modeled predicted results versus field observed values (i.e. head, contaminant concentrations, etc.).

2) A graphical presentation of head measurements and contaminant concentrations in the form of contour maps of observed and predicted values.

5.I INTERPRETATION OF RESULTS

The use of numerical models to simulate groundwater flow and contaminant transport systems has gained widespread acceptance in both government and industry. Yet, in spite of recent advancements in numerical modeling, the process provides only approximate values of output due to uncertainties in the input data and truncation error in the numerical solution schemes. As a consequence, the accuracy of the model output must always be critically evaluated.

The standard for evaluation of the modeled system should always be related to the degree of correlation between the simulation and the physical system. Modeling results also need to be evaluated to determine if they are physically reasonable. Other evaluations which need to be performed include:

1) An assessment of the uncertainty associated with the model results. In particular an assessment of the range of possible values for certain parameters should be presented.

2) An assessment of the limitations of the model. Particular emphasis should be directed toward addressing the utility of the model in predicting contaminant transport or attenuation, or to support decisions at sites where remedial designs or corrective actions are being considered.

3) An evaluation of possible errors associated with the modeling process. This assessment should include a discussion of error associated with the numerical solution of mathematical equations used in the model (ie:truncation errors, or round-off errors).

5.J CERTIFICATION

The above work shall be performed by or under the direct supervision of a Professional Geologist or Professional Engineer, registered in the State of Delaware. The professional's seal of certification must be affixed to the model submission document.

6. REFERENCES

California Department of Health Services. 1990. Technical Standards for the Mathematical Modeling of Ground Water Flow and Contaminant Transport at Hazardous Waste Sites, DRAFT.

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